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Supersonic reaction front propagation initiated by a hot spot in *n*-heptane/air mixture with multistage ignition

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ABSTRACT

For large hydrocarbon fuels such as *n*-heptane, multistage ignition occurs at low initial temperature. Therefore, multiple pressure pulses produced by multistage ignition and complicated reaction–pressure wave interactions are expected to happen during autoignition and reaction front propagation initiated by a hot spot. In this study, 1D simulations are conducted for *n*-heptane/air mixture with three ignition stages respectively caused by low-, intermediate- and high-temperature chemistries. Multiple pressure waves, shock waves, and detonation waves are identified and they are found to be generated by heat release from different ignition stages and reaction–pressure wave interactions. The thermal states of flow particles at different initial locations are tracked and analyzed; and the mechanism for the development of multiple shock waves and detonation waves is discussed. With the change of temperature gradient inside the hot spot or the hot spot size, such interactions can be strengthened or weakened and thereby the mode of supersonic reaction front propagation changes. Furthermore, both planar and spherical configurations are considered and the curvature effects are examined. It is found that in spherical configuration, the pressure wave caused by intermediate-temperature ignition is not strong enough to induce a second detonation wave as that in planar configuration.

1. Introduction

High compression ratio helps to improve thermal efficiency in spark ignition engines (SIEs) [1]. However, the tendency of knock increases greatly with compression ratio and currently knock is a severe constraint for downsizing SIEs with turbocharging [1–4]. Therefore, engine knock has received great attention recently [5–7]. It is generally accepted that knock in SIEs is caused by end-gas autoignition [1] and that the coupling between chemical reaction and pressure wave plays an important role in knock formation [5,8–10]. As mentioned by Wang et al. [10], "*knocking is still at an early stage of understanding*". Therefore, in order to understand knock mechanism, studies on various autoignition modes and reaction–pressure wave interaction are still needed.

Zel'dovich et al. [11,12] first analyzed different autoignition modes caused by non-uniform reactivity (i.e., a spatial distribution of ignition delay time). They found that detonation can develop at certain reactivity gradient. In the following decades, many studies were conducted to verify and to extend this theory using simplified one- or two-step kinetic models [13–17] or detailed reaction models [18–24]. More recenctly, Im et al. [54] have proposed a regime diagram for autoignition of homogeneous reactant mixtures with turbulent velocity and temperature fluctuations; and Grogan et al. [55] have developed an ignition regime diagram considering the competition between turbulent, chemical, and heat transfer effects in rapid compression machines. In these studies, the hot spot model with linear temperature distribution was popularly used and detonation was indeed observed at certain temperature gradient. However, only simplified chemistry models (one- or two-step chemistry) or simple fuels (such as H_2, CO and CH_4) were considered. Therefore, the chemistry considered in previous studies is greatly different from that of large hydrocarbon fuels used in SIEs, for which low-temperature chemistry and negative-temperature coefficient (NTC) phenomenon are involved.

In the literature, only a few studies considered autoignition and combustion modes of large hydrocarbon fuels with low-temperature chemistry. For examples, Ju et al. [25] investigated the ignition and flame propagation modes in *n*-heptane/air mixture and identified different combustion regimes caused by low- and high-temperature chemistries; Martz et al. [26] studied the combustion regime of a reacting front propagating into an auto-igniting *iso*-octane mixture; Sun et al. [27] found that low temperature ignition can cause strong pressure wave and flame oscillation in concentration-stratified *n*-heptane/air mixtures; and Im and coworkers [28–33] systematically examined the effects of turbulence and temperature inhomogeneity on autoignition processes of different fuels with/without low temperature chemistry. However, in all aforementioned studies, shock wave

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and detonation caused by reaction–pressure wave interaction were not observed. Only in our recent work [24], different supersonic autoignition modes including shock wave and detonation were identified for *n*-heptane/air mixture within the NTC regime. However, in [24] we did not focus on multistage ignition or its influence on modes of supersonic reaction front propagation for *n*-heptane/air at low initial temperature.

For large hydrocarbon fuels such as *n*-heptane, multistage ignition occurs at low initial temperature. Heat release during different ignition stages might produce different pressure pulses. Therefore, complicated reaction–pressure wave interactions are expected to happen. This was not investigated before and will be focused on in the present work. Although planar and spherical configurations were considered in previous studies, the geometry/curvature effects on supersonic reaction front propagation are still not well understood and will be examined here.

Therefore, based on above discussion, the objectives of the present study are two-fold. First, we investigate the supersonic reaction front propagation initiated by a hot spot in *n*-heptane/air mixture with multistage ignition. Pressure waves generated by different ignition stages are identified and their influence on modes of supersonic autoignition front propagation is examined. Second, we study the difference between ignition behaviors in planar and spherical configurations. The curvature effects in spherical configuration which weaken pressure waves and detonation waves are assessed.

It should be emphasized that the present work is different from [25] in three aspects: (1) in [25] a hot kernel of 1400 K was used to mimic spark assisted compression ignition while here a hot spot with linear temperature gradient is used to initialize the reaction front propagation; (2) as a result, supersonic reaction front was not observed in [25] while it is observed here; and (3) multiple pressure/shock/detonation waves generated by heat release from different ignition stages are identified and analyzed here through tracking the thermal states of flow particles at different initial locations while this was not found/conducted in [25].

The paper is organized as follows: in Section 2, the numerical model and methodologies are presented; then in Section 3, three ignition stages of *n*-heptane/air mixture at low initial temperature are identified and the critical temperature gradient is discussed; the interaction among different ignition stages and pressure waves as well as the geometry/curvature effects are investigated in Section 4; and finally, the conclusions are summarized in Section 5.

2. Numerical model and methodologies

2.1. Numerical model

In order to investigate the supersonic reaction front propagation and the interaction among different ignition stages and pressure waves, we simulate the transient autoignition process initiated by a hot spot for *n*-heptane/air mixture in a 1D closed chamber.

The transient autoignition process is simulated using the in-house code A-SURF [24,34,35]. A-SURF solves the conservation equations (including the unsteady Navier–Stokes equations as well as the energy and species conservation equations) for 1D, adiabatic, multi-component, reactive flow in a planar or spherical coordinate:

$$\frac{\partial U}{\partial t} + \frac{\partial F(U)}{\partial x} + N\frac{G(U)}{x} = F_v(U) + S_R \tag{1}$$

where N is the geometry factor ($N = 0$ and 2 for planar and spherical coordinates, respectively); and t and x are respectively the temporal and spatial coordinates (x should be replaced by r for spherical configuration). In Eq. (1), the vectors U, $F(U)$, $G(U)$, $F_v(U)$, and S_R are defined as:

$$U = \begin{pmatrix} \rho Y_1 \\ \rho Y_2 \\ \vdots \\ \rho Y_n \\ \rho u \\ E \end{pmatrix}, \quad F(U) = \begin{pmatrix} \rho u Y_1 \\ \rho u Y_2 \\ \vdots \\ \rho u Y_n \\ \rho u^2 + P \\ (E+P)u \end{pmatrix}, \quad G(U) = \begin{pmatrix} \rho u Y_1 \\ \rho u Y_2 \\ \vdots \\ \rho u Y_n \\ \rho u^2 \\ (E+P)u \end{pmatrix}$$

$$F_v(U) = \begin{pmatrix} -x^{-N}(x^N \rho Y_1 {V'}_1)_x \\ -x^{-N}(x^N \rho Y_2 {V'}_2)_x \\ \vdots \\ -x^{-N}(x^N \rho Y_n {V'}_n)_x \\ x^{-N}(x^N \tau_1)_x - N\tau_2/x \\ x^{-N} q_x + \Phi \end{pmatrix}, \quad S_R = \begin{pmatrix} \omega_1 \\ \omega_2 \\ \vdots \\ \omega_n \\ 0 \\ 0 \end{pmatrix} \tag{2}$$

In Eq. (2), ρ is the density, Y_k the mass fraction of species k, u the flow velocity, and E the total energy per unit mass. The subscript x in $F_v(U)$ stands for the partial derivative with respect to x. Instead of solving the continuity equation, the species conservation equations for all n species are solved in A-SURF. The continuity equation is recovered from the summation of all species conservation equations.

In the species conservation equations, ω_k and V'_k are the production rate and diffusion velocity of species k, respectively. The production rate ω_k is specified via collection of elementary reactions

$$\omega_k = M_k \sum_{j=1}^{n_r} \left\{ \left({\nu''}_{k,j} - {\nu'}_{k,j}\right) \left[K_{f,j} \prod_{k=1}^{n} \left(\frac{\rho Y_k}{M_k}\right)^{{\nu'}_{k,j}} - K_{b,j} \prod_{k=1}^{n} \left(\frac{\rho Y_k}{M_k}\right)^{{\nu''}_{k,j}} \right] \right\} \tag{3}$$

where M_k is the molecular weight of species k; n_r is the total number of elementary reactions; $\nu'_{k,j}$ and $\nu''_{k,j}$ are the molar stoichiometric coefficients of species k in reaction j; and $K_{f,j}$ and $K_{b,j}$ are the forward and reverse reaction rate of reaction j. The forward reaction rate for each elementary reaction is usually modeled using the empirical Arrhenius law

$$K_{f,j} = A_{f,j} T^{\beta_j} \exp\left(-\frac{E_j}{RT}\right) \tag{4}$$

where A_{fj} is the pre-exponential constant, β_j the temperature exponent, and E_j the activation energy. The reverse reaction rate can be obtained from chemical equilibrium constant and the forward reaction rate. These parameters (A_{fj}, β_j, E_j) are given in the chemical mechanism and the reaction rates are calculated using the CHEMKIN package [36].

In simulation we use the skeletal mechanism for *n*-heptane oxidation [37]. It consists of 44 species and 112 elementary reactions. This mechanism has been demonstrated to be able to accurately predict ignition (including the NTC regime) and flame propagation in *n*-heptane/air mixtures at a broad range of temperature and pressure [37].

The diffusion velocity of species k is composed of three parts:

$$V'_k = V'_{k,Y} + V'_{k,T} + V'_{k,C} \tag{5}$$

$V'_{k,Y}$ is the ordinary diffusion velocity given by the mixture-averaged formula [38]:

$$Y_k V'_{k,Y} = -D_{km} \frac{1}{\bar{M}} \frac{\partial (Y_k \bar{M})}{\partial x} \tag{6}$$

where D_{km} is the mixture-averaged diffusion coefficient of species k and $\bar{M}$ is the mean molecular weight of the mixture.